Enhanced Analysis for Pulsed Voltammetry Evaluation Tool / System for Improved Power Systems

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The official link for this solicitation is:
http://www.acq.osd.mil/osbp/sbir/solicitations/sbir20152/index.shtml

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Description:
In order to develop new high-performance batteries, fuel cells, and sensors, the electrochemical behavior of materials and devices need to be quantitatively assessed. This assessment (models and systems characterization) will help identify the performance of electrochemical systems leading to the development of significantly improved power sources. New electrochemical analysis tools will enable better characterization of electrodes, electrolytes, and devices. Often only a few data points from a voltammogram or working curves for each experimental condition are used to determine, the formal potential and peak current. These analyses can be imprecise due to background currents, multiple redox processes, etc. Pulse voltammetry not only reduces charging currents but can also be mathematically described and modeled. To date a limited set of fundamental models have been developed to describe the pulsed voltammetric response for complex mechanisms and electrode geometries using the data contained in the complete voltammogram. Additional models need to be developed and these techniques made accessible to the research community using a generalized approach that can easily determine relevant electrochemical parameters from datasets obtained by modern instrumentation. In particular, it is not possible to determine the reversible half-wave potential, the charge transfer coefficient, the heterogeneous charge transfer rate, or the diffusion coefficient from the entire voltammogram. A tool is needed that is able to quantify electrochemical parameters using a variety of pulse profiles and would enable enhanced understanding of the behavior of redox couples and resultant devices such as batteries, fuel cells, and electrochemical

sensors. Furthermore, the algorithms must be able translate between different types of instrumentation and new pulse based voltammetry techniques. These tools would be integrated into commercial electrochemistry data generation and analysis packages. PHASE I: Develop models and measurement / characteristic tools that can determine reversible half-wave potential, the charge transfer coefficient, the heterogeneous charge transfer rate, and the diffusion coefficient for single square wave voltammograms. The resultant tool should allow the parameters to be calculated entirely from the voltammograms (with user provided initial values) or allow individual variables to be set by the user and the other variables calculated based on the voltammogram. In addition, the package should determine the confidence/uncertainty for the calculated electrochemical parameters. PHASE II: Incorporate additional models to allow utilization of data from a variety of pulse voltammetry techniques including: normal pulse, reverse pulse, and differential pulse voltammetry, as well as coupled electrochemical and chemical mechanisms such as preceding chemical reaction, following chemical reaction, catalytic chemical reaction, etc. The algorithm should also be capable of determining the electrochemical parameters from a "bundled" series of voltammograms with for example varying square wave frequency. Verify with statistical confidence intervals the accuracy of the data obtained. Integrate the models and evaluation tools into commercial electrochemistry data generation and analysis package that will assist in determining prospective solutions performance. PHASE III: This product would be used in a broad range of military and civilian research with applications including: advanced batteries, electrosynthesis, electrocatalysis, and detectors to provide decisions on which technologies to further develop for improved electrochemical power sources.